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Periodizing transformations for numerical integration

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Abstract

The order of the trapezoidal rule can be raised by making a substitution that transforms the integrand into a new integrand which has a smooth periodic extension. The exponent in the rate at which the transformed weights approach zero near the endpoints is called the *damping power* of the transformation. Currently used polynomial transformations of damping power m have order $m+1$ if m is odd, and order $m+2$ if m is even. We prove that the highest possible order is $m+1$ if m is odd, but $2m+2$ if m is even, and give new polynomial transformations that achieve the optimal order.

Keywords: Integration; Periodic; Transformation

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1. Introduction

The most primitive numerical methods for the calculation of an integral

$$If = \int_a^b f(x)\,dx \tag{1}$$

are the trapezoidal rule

$$T_h f = h\left(\tfrac{1}{2}f(a) + \sum_{j=1}^{n-1} f(a+jh) + \tfrac{1}{2}f(b)\right) \tag{2}$$

and the midpoint rule

$$M_h f = h\sum_{j=1}^{n} f\left(a + (j-\tfrac{1}{2})h\right), \tag{3}$$

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where $h=(b-a)/n$ for some natural number n. It is convenient to work with the indefinite integral

$$F(x)=\int f(x)\,\mathrm{d}x \tag{4}$$

even though it is unknown in practice. An asymptotic expansion (the Euler–Maclaurin summation formula) for the error in the trapezoidal rule is given by

$$If-T_hf\sim\sum_{k=1}^{\infty}B_kh^{2k}\left(F^{(2k)}(b)-F^{(2k)}(a)\right), \tag{5}$$

where the constants B_k are known in closed form (see e.g. [1]) but do not concern us here. The same expansion, but with other constants, holds for the midpoint rule.

As is usual with asymptotic expansions, (5) should not be seen as a convergent series; the interpretation is rather that if p is the lowest index for which $F^{(2p)}(x)$ exists and is continuous for all $x\in[a,b]$, but $F^{(2p)}(b)\neq F^{(2p)}(a)$, then

$$If-T_hf=B_ph^{2p}\left(F^{(2p)}(b)-F^{(2p)}(a)\right)+\mathrm{o}(h^{2p}), \tag{6}$$

where as usual $\mathrm{o}(h^{2p})$ means a quantity that tends to zero faster than h^{2p}. In this case, we say that the trapezoidal rule is of *apparent order* $2p$ for the integrand f. Note that the definition of apparent order depends on the integrand. If we say that a quadrature rule has order q, it means that for all integrands f such that $f^{(q)}(x)$ exists and is continuous for all $x\in[a,b]$, the formula is of apparent order at least q, and for at least one such integrand, it is of apparent order no greater than q. Thus, the trapezoidal rule has order 2.

In this paper, we are concerned with substitution methods that are used to "preprocess" the integrand in order to raise the apparent order. We use the familiar analytical tool of making the substitution $x=x(t)$ so that

$$If=\int_{t_a}^{t_b}f(x(t))x'(t)\,\mathrm{d}t=\int_{t_a}^{t_b}F'(x(t))\,\mathrm{d}t, \tag{7}$$

where

$$x(t_a)=a; \qquad x(t_b)=b. \tag{8}$$

We shall assume that x is a monotonic function of t, and that $[a,b]=[t_a,t_b]=[0,1]$. In that case, x can be represented by

$$x(t)=\frac{\int_0^t w(s)\,\mathrm{d}s}{\int_0^1 w(s)\,\mathrm{d}s}, \tag{9}$$

where the *weight function* w is nonnegative and not identically zero. We denote the positive number $\int_0^1 w(s)\,\mathrm{d}s$ by K_w. In addition, we restrict our attention to *symmetric* transformations where the weight function satisfies $w(t)=w(1-t)$ for $0\leqslant t\leqslant 1$. When w is suitably chosen, the trapezoidal rule is of higher apparent order for the integrand G', where $G(t)=F(x(t))$, than for the original integrand F'.

Although it is not hard to construct cases where for a particular integrand one obtains $G^{(2p)}(t_b)=G^{(2p)}(t_a)\neq 0$, in general the only way of guaranteeing a higher order is to choose x so that some derivatives of G necessarily vanish at both endpoints. Many substitutions have been suggested that send all derivatives to zero: see [6] for a survey. Less well studied are transformations that send only a finite number of derivatives to zero. These transformations have been applied mainly in multidimensional integration [2–4]. In this paper, we analyze the polynomial transformations that have been applied by these authors, and introduce some new polynomial transformations that are optimal in a sense to be defined in Section 4.

A typical property of weight functions is that they vanish together with some of their derivatives at the endpoints of the interval. We shall say that a weight function is of *damping power m* if in a neighbourhood of $t = 0$,

$$w(t) \sim Ct^m, \tag{10}$$

where C is a nonzero constant. It is undesirable to use a transformation with too much damping power, because the weights of many of the transformed points become so small that they no longer contribute significantly to the integral, thus in effect reducing the number of points.

Sidi [9] defines a class $\mathcal{S}_m$ of transformations by the property that a weight function of damping power m is in $\mathcal{S}_m$ if its Maclaurin series contains only terms of the same parity as m (i.e. if m is odd, the series contains only odd powers of t, etc.) An example of a transformation in $\mathcal{S}_m$ is

$$w(t) = (\sin \pi t)^m. \tag{11}$$

He proves various theoretical properties of transformations in $\mathcal{S}_m$, including the property that the transformations are of optimal order when m is even but not when m is odd, and remarks: "It would be interesting to know whether there are further variable transformations in $\mathcal{S}_m$ that can be expressed in terms of elementary functions as the $\sin^m$-transformation. So far we have not been successful in constructing such a transformation." In Theorem 2 we show that the class $\mathcal{S}_m$ is a little too restrictive, in the sense that for even m, the terms above t^{2m} in the Maclaurin series of $w(t)$ do not influence the order. Indeed, our polynomial transformations that satisfy the conditions of Theorem 1 do not belong to $\mathcal{S}_m$.

The main tool used in this paper is the formula of Faà de Bruno [7, 8], which states that when $G(t) = F(x(t))$, the kth derivative of G is given in terms of the derivatives of F and x by

$$G^{(k)}(t) = \sum_J d_J F^{(\sigma(J))}(x) \prod_{i=1}^{\sigma(J)} x^{(j_i)}(t) \tag{12}$$

where the sum ranges over all partitions $J = (j_1, j_2, \ldots, j_\sigma)$ of the integer k, and $\sigma(J)$ denotes the number of parts, i.e.,

$$\sum_{i=1}^{\sigma(J)} j_i = k. \tag{13}$$

The constants d_J are known in closed form [7, 8] but do not concern us here: it is enough to know that they are all positive.

2. Korobov's polynomial transformations

A family of polynomial transformations first given by Korobov [5] is obtained by choosing

$$w(s) = (s(1-s))^m \tag{14}$$

in (9), where m is a nonzero integer: the case $m=0$ amounts to making no transformation. Note that $w(s)$ is symmetric around $s=\frac{1}{2}$. These transformations are popular among practitioners of lattice rules: the case $m=1$ is used as a periodizing transformation in all the numerical experiments given in [4]; the case $m=4$ is similarly used in [3]; the cases $m=2,4,5,6,7$ appear in [2].

Unfortunately, the transformation (14) does not raise the order of the trapezoidal rule when $m=1$. For the case $k=2$ we find from (12) that

$$F''(t) = d_{1,1}F''(x)\left(x'(t)\right)^2 + d_2F'(x)x''(t) \tag{15}$$

and since $x''(t)$ is a multiple of $w'(t)$, which is nonzero at the endpoints, we cannot expect $F''(b)-F''(a)$ to be zero in general.

When $m=2$, the order of the trapezoidal rule is indeed raised, since w' is zero at both end points. Since by (6) the order must be an even number, we apply the formula (12) for $k=4$. The term containing d_4 involves w''', which is nonzero: hence the order is 4.

The general case is covered by the following theorem.

Theorem 1. *The order of the trapezoidal rule transformed by the Korobov transformation* (14) *is* $2p$ *where* $p=\lceil(m+1)/2\rceil$.

Proof. The order is given by the lowest even derivative $G^{(2k)}(t)$ that is nonzero at $t=0$, because by the symmetry of w, all lower derivatives vanish at both endpoints. Note that the expansion of $w(s)$ is a linear combination of the powers s^j in the range $m\leqslant j\leqslant 2m$, with all coefficients nonzero. Therefore the derivatives $w^{(j)}(0)=K_w x^{(j+1)}(0)$ are nonzero for $m\leqslant j\leqslant 2m$ and zero otherwise. The term in the expansion (12) containing d_{2p} involves $x^{(2p)}$, and therefore the order $2p$ is the smallest even number greater than or equal to $m+1$. $\square$

Another way of stating this theorem is: for even values of m, the transformation has order $m+2$, but for odd values of m the transformation is of order $m+1$. There is therefore no great advantage to be gained by choosing an odd value of m: the immediately preceding even value yields the same order.

To illustrate this conclusion, we give a simple numerical example, where the integrand is $f(x)=e^x$. This integrand has the desirable property that each of its derivatives is positive, but assumes unequal values at the endpoints; thus the possibility that a term in (12) fortuitously vanishes is avoided. The integrand was transformed by the transformation (14) with the exponent m ranging from 0 (no transformation) to 7, and the trapezoidal rule (2) with n ranging from 12 to 80 was applied. In Table 1 we give the approximate order $2\tilde{p}$ of the transformed trapezoidal rule, obtained by estimating the slope on a log–log plot of the error versus the step size; the actual order $2p$, which is the even number closest to $2\tilde{p}$; and the constant c_m in the approximation error $\approx c_m h^{2p}$, also obtained from the log–log plot, but with the actual order $2p$ taken as fixed. The computations were made using double precision (approximately 16 decimal digits): since the actual error for $m=7$ and $n=80$ is approximately 10^{-13}, it would require higher precision to extend the table beyond $m=7$.

We make the following observations about Table 1:

- The agreement between the numerically obtained order $2\tilde{p}$ and the actual order $2p$ is very close, and confirms the theoretical result.

Table 1
The error in the trapezoidal rule combined with the polynomial transformation (14) is approximately $c_m h^{2p}$

m	$2\tilde{p}$	$2p$	c_m
0	1.99996	2	−0.1431
1	2.00034	2	1.8603
2	3.99737	4	1.8475
3	3.99643	4	−4.3009
4	5.99765	6	−36.9612
5	5.97395	6	38.2119
6	7.985	8	1073.1
7	7.899	8	604.9

- When m is odd, the transformation has the same order as the transformation using the even exponent $m-1$, but as m becomes larger, the error constant for odd exponents does not increase as fast as that for even exponents.
- The transformation with $m=1$ is actively harmful, as can be seen by comparing c_1 to c_0, and amounts to sacrificing a full decimal digit of precision.

3. Bounds on the order of the transformed trapezoidal rule in terms of damping power

In the preceding section, we saw the polynomial transformations (14) of damping power m have order $m+1$ when m is odd and $m+2$ when m is even. In this section, we answer the question: what is the highest order that a transformation of given damping power can have?

Theorem 2. *If the trapezoidal rule is transformed by*

$$x(t)=\frac{\int_0^t w(s)\,\mathrm{d}s}{\int_0^1 w(s)\,\mathrm{d}s},$$

where $w(t)=w(1-t)$ and $w(t)\sim ct^m$ for some nonzero constant c in a neighbourhood of $t=0$, then for odd m the order of the transformed rule is always $m+1$, but for even m, the order can be as high as, but no higher than, $2m+2$. The latter case is achieved if and only if w satisfies the conditions

$$w^{(j)}(0)=w^{(j)}(1)=0, \quad j=0,1,\ldots,m-1; \tag{16}$$

$$w^{(j)}(0)=w^{(j)}(1)=0, \quad j=1,3,\ldots,2m-1. \tag{17}$$

Proof. Note that $x^{(m+1)}(0)=w^{(m)}(0)\neq 0$. Therefore, for odd m, the term involving d_{m+1} in the evaluation of formula (12) for the even derivative $G^{(m+1)}$ is nonzero, and the order is $m+1$.

For all values of m, the term involving $d_{m+1,m+1}$ in the evaluation of formula (12) for $G^{(2m+2)}$ is nonzero, and the order can therefore be no greater than $2m+2$. This argument also shows that the conditions (16) are necessary.

Consider the formula (12) for an even derivative $G^{(2k)}$ with $k \leqslant m$. Since $x^{(2k)} = w^{(2k-1)}/K_w$, the term involving d_{2k} is zero at both endpoints if and only if the conditions (17) hold.

All other partitions of $2k$ involve at least two pieces, of which no more than one can exceed k. Therefore, the term corresponding to such a partition contains a derivative $x^{(j)}$ with $j \leqslant k \leqslant m$. Since $x^{(j)} = w^{(j-1)}/K_w$, all those derivatives are zero at both endpoints when $j \leqslant m$ if the conditions (16) hold, and we then have $G^{(2k)} = 0$ for $k \leqslant m$, which implies that the order is $2m+2$.

It is sufficient to exhibit one function that satisfies the conditions (16) and (17). Such a function is $w(t) = (\sin \pi t)^m$. $\square$

4. Optimal polynomial transformations

With the aid of the theory of the preceding section, we now introduce some new polynomial transformations that are claimed to be better than the Korobov transformations.

We call a polynomial transformation optimal if it has damping degree m, order $2m+2$, and the polynomial w is of lowest possible degree. There are $3m$ equations in (16) and (17), and therefore we need a polynomial of degree $3m$ in order to produce a nontrivial solution to these equations. It simplifies matters to think of w as a polynomial of degree $\frac{3}{2}m$ in the variable

$$u(t) = t(1-t). \tag{18}$$

Clearly w must contain the factor u^m. With the aid of a computer algebra package, we found the following solutions:

$$\begin{aligned} m = 2:&\quad w(t) = u^2(1+2u),\\ m = 4:&\quad w(t) = u^4(1+4u+6u^2),\\ m = 6:&\quad w(t) = u^6\left(1+6u+\frac{903}{58}u^2+\frac{538}{29}u^3\right). \end{aligned}$$

To obtain x, we make the ansatz that the indefinite integral of w can be written as

$$\int w(t)\,\mathrm{d}t = -u'(t)p(u).$$

where p is a polynomial. Differentiating, we obtain

$$\begin{aligned} w(t) &= -u''(t)p(u) - (u'(t))^2 p'(u)\\ &= 2p(u) + (4u-1)p'(u). \end{aligned}$$

If we express w and p in the form

$$\begin{aligned} w(t) &= b_0 + b_1 u + \cdots + b_M u^M,\\ p(t) &= p_0 + p_1 u + \cdots + p_M u^M, \end{aligned}$$

where $M = \frac{3}{2}m$, a comparison of coefficients yields

$$b_j = (4j+2)p_j - (j+1)p_{j+1}, \quad j = 0,1,\ldots,M, \tag{19}$$

where $p_{M+1} = 0$. Eqs. (19) can be solved by backwards recurrence.

In the case $m = 2$, this method yields

$$x(t) = \tfrac{1}{2} + (2t - 1)(\tfrac{1}{2} + u + 3u^2 + 3u^3). \tag{20}$$

Claus Schneider (personal communication by electronic mail) has found an analytic representation in terms of Bernoulli polynomials for the transformation function x for all even values of m, thereby proving its existence. He has also proved that any polynomial w of degree $3m$ that satisfies the conditions (16) and (17) must be nonnegative in the interval $[0, 1]$, thus producing a monotonic transformation x.

When we apply the transformation (20) to the test example of Section 2, the approximate order $2\tilde{p}$ is 5.9752, and numerically we find that the error is approximately $0.8027h^6$. This error is nearly 50 times smaller than that of the Korobov transformations of order 6 obtained by taking $m = 4$ and $m = 5$ in (14). For the order 6 transformation

$$x(t) = t - \frac{1}{2\pi}\sin(2\pi t). \tag{21}$$

obtained by taking $m = 2$ in (11), the apparent order is 6.0135, and numerically we find that the error is approximately $-0.9173h^6$. This value is a little larger than that of the optimal polynomial transformation of damping power 2.

5. Repeated transformations

A quick device for obtaining a transformation of higher order is to repeat a known transformation, i.e., use the transformation $x(x(t))$. The order of the repeated transformation can be read off from the Maclaurin series of $x(x(t))$: it is the smallest even number that can be expressed as a sum of exponents appearing with nonzero coefficients in the series. That means either the lowest even exponent, or twice the lowest odd exponent, whichever is least.

For example, the Maclaurin series for the optimal polynomial transformation of damping power 2 has the form

$$x(t) = k_3t^3 + k_5t^5 + k_6t^6 + \mathrm{O}(t^7).$$

Therefore,

$$\begin{aligned} x(x(t)) &= k_3(x(t))^3 + k_5(x(t))^5 + k_6(x(t))^6 + \mathrm{O}((x(t))^7) \\ &= l_9t^9 + l_{11}t^{11} + l_{12}t^{12} + l_{13}t^{13} + l_{14}t^{14} + \mathrm{O}(t^{15}). \end{aligned}$$

The nonzero exponents less than 15 all come from the expansion of $(x(t))^3$ and all the numbers are of the form $i + j + k$ where $i, j, k \in \{3, 5, 6\}$. The even exponent $12 = 3 + 3 + 6$ determines the order of the repeated transformation. This repeated transformation is not optimal, since an optimal transformation with damping power 8 would have order 18.

Sidi [9] shows that compounding two transformations in $\mathcal{S}_m$ yields another transformation in $\mathcal{S}_m$. It therefore follows by an analysis similar to the above that repeating a transformation in $\mathcal{S}_m$ raises the damping power from m to $m(m + 2)$ and the order from $2m + 2$ to $2(m + 1)^2$.

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